Sailors: a Simulator for a Shaft for Direct Reduction of Iron Ore

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Direct Reduction (DR) is an alternative route for the production of steel based on the use of a mixture of natural gases. DR has been investigated within SP12 and in this framework a model for the simulation of the reduction of burden material in the shaft has been developed and a stand-alone software has been realized. The results obtained by the model show a very good agreement with real data collected from existing plants and could be used in the designing phase of DR plants.

Introduction

Direct reduction (DR) is an alternative route for the production of steel which has been developed in the last years. This process allows the production of Direct Reduced Iron by means of a mixture of reducing gases mainly composed by hydrogen and carbon monoxide which play the role of reducing agents.

The main part of the DR plant is the reduction shaft where the reduction reactions take place. During the production the shaft is charged from the top with iron ore and the reducing gas are blown from the bottom in order to allow the reduction while the produced DRI is collected from the bottom of the shaft.

In this paper it is proposed a model developed in order to simulate the reduction process which takes place in the reduction shaft of a DRI production plant. In particular, given the geometry of the shaft, the composition, temperature and pressure of the inflated gas, the model estimates the hourly DRI production that can be obtained by using a specified burden material. The reduction kinetics of the burden material is a fundamental information for the model and is characterized by means of another model named IRES (see Sec. 1), which is based on a series of laboratory tests carried out on the material.

The developed model, described in part 2, in order to be easy to use, has been implemented in a stand-alone application realized in Visual basic that combines a user-friendly interface and high computation capabilities. The developed software tool is described in Sec. 3.

Finally the SAILORS model has been tested in order to evaluate the accuracy of the produced simulations. For this purpose the results obtained by the model on a set of known shaft configurations and burden materials have been compared with measured values available from literature. The obtained results presented in Sec. 4, are encouraging and clearly demonstrate the goodness of the SAILORS model.

Part 1. SAILORS background: burden material reduction behaviour characterization and reduction simulations

SAILORS is a one-dimension finite element model. It is based on a subdivision of the shaft in 50 overlapping elements of the same diameter of the shaft. It is assumed that in each element the conditions affecting material reduction can vary along the axes of the cylinder and not along its radius. The reduction of burden material which takes place within each layer is simulated by using the IRES model.

IRES (Ilva REduction Simulation) is a model for simulating the reduction behavior of an arbitrary material depending on temperature and gas composition, provided that a set of kinetic characteristics related to the material have been determined through laboratory tests.

The general kinetic laws obtained from tests performed at constant conditions of temperature and gas composition have been subsequently validated by means of other tests performed at variable temperature and gas composition conditions. For the characterization of a material various isothermal reducibility tests have been run at different temperatures and different reducing gas compositions. During the tests, the weight loss was continuously registered and subsequently converted into reduction percentage (indicated with R in the following). The variability ranges of conditions affecting reduction as well as some parameters of lab tests are listed in table 1, while some sample test results are shown in Figure 1. As it can be seen in table 1, tests refer to typical DRI conditions [3]. The pellets used for the tests were provided by one project partner and they belong to the common types of pellets used in DRI plants [4]. Based on the results of the experiments, the kinetic laws of the reduction reaction have been assessed. The following general kinetic law has been considered:

$$R(t) = 100.(1 - e^{-Kt}) \qquad (1)$$

Parameter	Min	Max
Temperature	700°C	900°C
H_2	45%	85%
CO	7%	48%
CO_2	2.5%	4.5%
Gas speed (STP)	0.057 m/s	
Gas flow (STP)	9.21 l/min	
Reduction section diameter	59 mm	
Initial sample weight	307 g	
Pellet size	12.5 mm	15 mm

Table 1. This table summarizes the variability of the test conditions for the main parameters

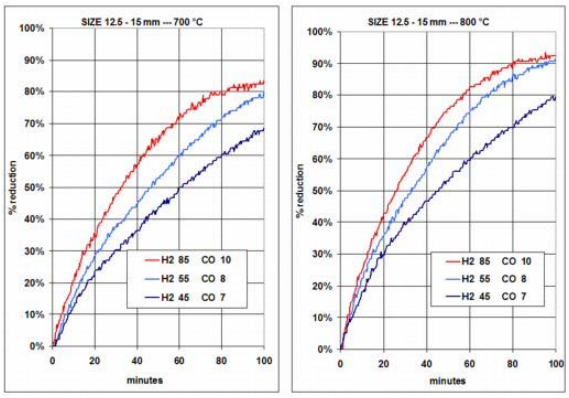

Figure 1. Sample results of the performed reduction tests. These tests have been carried out at constant temperature and gas composition

where t is the time and K is the kinetic factor depending on the material type and size, the reducing environment and the temperature. The process of correlating the experimental results with the main test conditions (temperature, gas composition...) has undergone various and different stages. As a conclusion it was found that:

- the reduction behaviour of all materials tested can be adequately described by equation 1
- the gas composition can be represented by introducing the concept of *equivalent % CO content*: 1 mole of H_2 = 2 moles of CO (so that, for instance, 50% CO + 10% H_2 behaves as 70% CO)
- The parameter K can be linearly correlated to the gas composition and temperature, i.e. $K = a \cdot x + b$, where: a and b are constants to be determined by fitting the experimental results and X is a parameter defined as: $X = \left(\frac{T}{1000}\right)^{2.5} \frac{[CO_2]eq}{1000}$ where T is the absolute temperature and $[CO]_{eq}$ is the percentage of equivalent CO.
- Usually the root mean square error between actual test data and those obtained from the above correlation lies within a few %.

In Figure 2 a simulation of material reduction is compared to its measured behavior showing the good performance of the model for isothermal and constant gas composition tests. The shown simulation refers to an extreme situation within given test ranges and highlights the goodness of the proposed fitting also for borderline conditions.

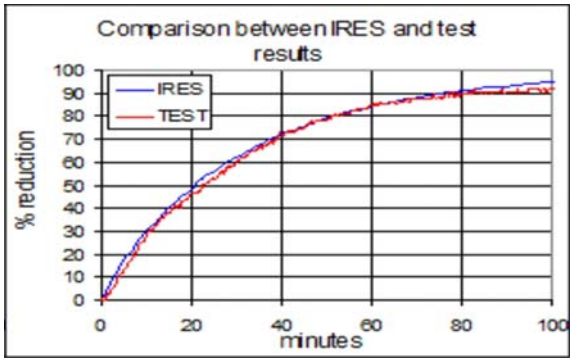

Figure 2. Comparison between a laboratory test and its IRES predicted behavior

The kinetic parameters determined through the above described tests are stored in a database which describes the reduction behavior of several materials at different conditions. Such parameters are used to simulate the reduction of the tested materials as well as mixtures of them for varying temperature and gas composition in order to be in line with the conditions of the DRI production shaft.

Varying conditions are simulated by considering any temperature-gas profile as a sequence of steps whose duration is sufficiently short to be assumed as isothermal and with constant gas composition. Moving from a step to the following one requires the concept of *virtual time* i.e. the time required to reach under an hypothetical history with the temperature and gas composition of the next step, the same reduction index already reached during the real history. The extra reduction gained in the subsequent step is equivalent to that which would be obtained in a step of equal duration beginning at *virtual time*.

The concept is better described in picture 3 which refers to a 2 steps history: the first one consisting of a 100 minutes reduction time with 20% CO followed by 100 minutes with 50% CO.

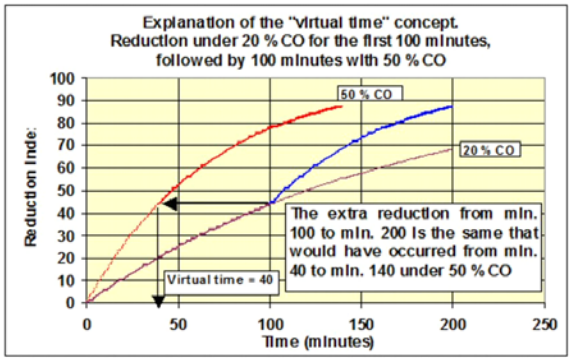

Figure 3. Explanation of the "virtual time" concept

Part 2. The SAILORS model

IRES is used within the SAILORS model playing the role of *reduction module* for a more general model designed to simulate the shaft of a direct reduction furnace. In particular IRES is used to simulate the reduction of burden material in each element of the 1-Dimension finite element model.

The main assumptions considered for the development of the model are as follows:

- In order to exploit finite element simulation the shaft is divided in 50 cylindrical overlapping elements. In each elements conditions are assumed to vary only along the axe of the cylinder but not along its radius. Elements are numbered 1 to 50 starting from the bottom.
- Reducing gas and burden material move in opposite direction: gas enters from the bottom of the shaft while material is put in from the top.
- Reducing gas is formed by: H_2, H_2O, CO, CO_2

A scheme of the described shaft including input and output of gases and materials is shown in Figure 4.

The main inputs needed by the model, corresponding to the main variables of the shaft, are the following:

- Dimension of the reduction shaft (height and diameter)
- Flow rate, composition, temperature and pressure of inlet gas
- Inlet burden material temperature
- Target reduction of outlet material

On the other hand the model will provide the following outputs:

- Produced DRI outlet flow
- Temperature profile for both gas and material in the shaft
- Reduction profile of material in the shaft

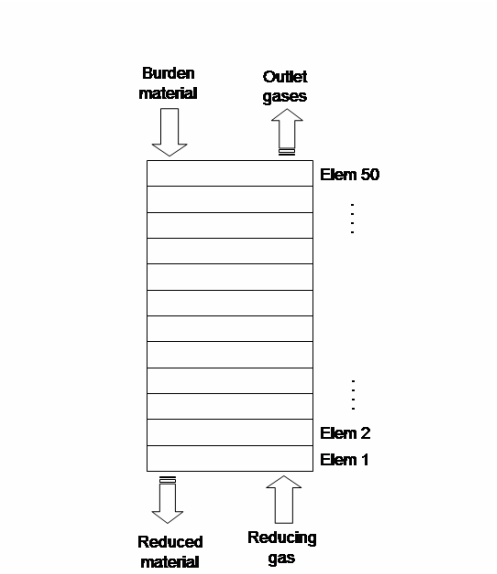

Figure 4. The scheme of the shaft utilized by the SAILORS model

Within the finite element model in each layer forming the shaft several physical process and relations among variables are considered. In this framework all reactions are heavily influenced by the composition of reducing gas. From the thermal point of view there is heat exchange between gas and material (gas cools as it gets high in the shaft and material gets warmer as it goes down). From the chemical point of view, gas reduces the mineral by subtracting oxygen which combines with H_2 and CO and forms CO_2 and H_2O. Such reactions lead to an energy exchange which must be taken into consideration (for instance the reaction with H_2 absorbs energy while the one with CO releases energy).

The functioning of the 1-dimension finite element model managing these thermal and chemical-physical interactions can be described by the following points:

1. A first simulation of reduction is carried out, by ignoring all thermal exchanges but assigning an arbitrary initial temperature value to the burden material. The simulation, through an iterative process based on the use of the IRES model, calculates an inlet material flow which is compatible with the target reduction.
2. Given the inlet material flow calculated in the previous step, the thermal balance is calculated in order to obtain the temperature of gas and material in each layer the shaft is divided in. To this purpose both the thermal balance within each layer and boundary conditions must be taken into ac-

count. In particular, two boundary conditions have to be respected: the first one for the upper border concerning inlet material whose temperature is known; the other one on the lower border concerning inlet gas temperature which is known as well.

3. Given the thermal profiles calculated in step 2 a new inlet material flow is calculated as in step 1 but in this case new thermal conditions will be exploited. The computation ends when the calculated inlet material flow value is stabilized according to a set of convergence criteria established by the user.

The calculation process described above is shown by means of a flow chart in Figure 5.

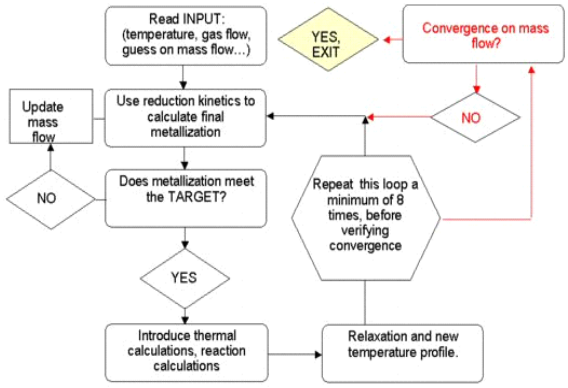

Figure 5. Block diagram describing the SAILORS model flow

Within the simulation IRES is used for the inlet material flow calculation. Material flow calculation starts from element number 1 and goes on element by element from the bottom to the top of the shaft. In such situation and at each step the material temperature is known (from the current thermal profile) as well as the gas composition in the shaft element, the reduction degree on the bottom of the element and the residence time of mineral in the element. IRES is used each time to calculate the reduction degree on the top border of the considered element which represent the reduction degree of mineral in a previous moment as the mineral goes from the top to the bottom of the shaft. To this purpose, IRES calculates the reduction profile of the material until the reduction of the mineral at the exit of the element is reached under the conditions of temperature and gas composition of the considered element, then it looks backward of a time t which represents the residence time of material in the element. The obtained result is the reduction degree of material once it enters the element. The reduction degree of 50th element is used in order to verify the mass balance for the current situation: if there is convergence the calculation can stop, otherwise parameters are modified until convergence is reached.

Part 3. The developed software

On the basis of the above described 1D finite element model a software for the DR simulation was implemented. It was decided to realize a stand alone application for two main reasons: the first one is related to the complexity of mathematics involved in the calculus and to the heavy computational burden. Such computational effort needs to be afforded by a dedicated software expressly designed and compiled in order to minimize the computational time. The second reason is related to the necessity of having a user friendly software which makes the selection and modification of the numerous parameters involved in the simulation easy and provides a clear visualization of results.

For the implementation of the software Microsoft© Visual Basic was chosen because it gives at the same time the possibility of:

1. writing code to be compiled by the standard VB compiler. The code compilation gives the advantage of creating a portable stand alone software compatible with MS Windows© based systems. Moreover the compilation drastically increases the speed of the whole computation.
2. designing in a very natural way a user friendly interface similar to most software running under Microsoft operative systems
3. easy interfacing with other programs used for the loading and storage of data used by the model

The software has been implemented by using several modules, each one performing a particular operation or set of operations, in order to facilitate subsequent modifications or code addictions: there are for instances procedures for the mass balance, for the thermal balance and some for the management of finite element modelling engine.

The main interface window of the developed software is shown in Figure 6 and includes a zone for the input of plant and materials parameters in which main properties of the shaft and the burden material are chosen and an output area for the monitoring of main information concerning each of the 50 elements in which the shaft is divided and the main results of the DRI simulation; moreover a picture showing the progress of reduction and temperature of the material and reducing gas inside the shaft is included.

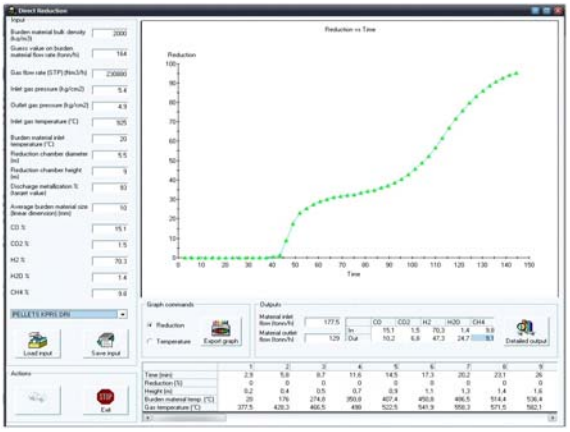

Figure 6. The main window of the developed interface

The complete list of the inputs to the model inserted through the interface and taken into account by the model is the following:

- material bulk density
- guess value on burden material flow rate (needed for the finite element algorithm)
- gas flow rate
- inlet gas pressure
- outlet gas pressure
- burden material inlet temperature
- reduction chamber height
- reduction chamber diameter
- target discharge metallization
- average burden material size
- inlet gas composition
- burden material type

In addition to these inputs, when a burden material is chosen for the simulation, the software exploits some information previously stored in a separate (independent and editable) Excel file. This file contains information used by the IRES model embedded in SAILORS and describes the kinetic of the reduction of the specific material. The list of burden materials can be extended by simply adding information to the Excel file and in an analogous manner material properties can be modified.

SAILORS allows the user to save and subsequently recall an input set in order to form a library of principal input situations.

The software, after the calculation is complete, returns the following information on the main window:

- material inlet flow
- material outlet flow
- outlet gas composition
- for each element of the shaft: gas temperature, burden temperature, reduction rate, residence time (in a table)

When the calculation is completed the picture area is updated and it is possible to show both a graphic describing the progress of reduction rate in function of time or (by selecting the specific radio-button) the burden and gas temperature in function of the height of the shaft. It is also possible to export these figures in the JPG format. More detailed data are available by accessing a further window which provides the following information:

- total production rate of reduced material
- metallization degree
- total iron
- total metallic iron
- residence time
- oxides
- total oxygen transferred

All the above described output data can be exported in a plain ASCII file easily readable by most common text editors. The so exported file will include also information concerning the input parameters of the simulation.

The computation time is in line with the expectations. A single run of the simulation depends on the whole set previously mentioned parameters. Normally simulations on a 2.4GHz processor computer with 2GB ram takes from 5 to 20 seconds.

Part 4. Numerical results

In order to validate the developed model, some real data coming from the most common DRI production plants have been compared with the corresponding simulations performed by SAILORS. Such information are confidential and come from the work carried out within the ULCOS project. In particular tests refer to a set of different configurations both for the dimension of the shaft and for other parameters such as inlet gas composition and temperature while the used burden material is for all tests the same kind of commercial pellets. The variability of such parameters, whose ranges are shown in table 2, is important as it has allowed to test the simulator in a wide range of conditions

The real plant hourly DRI production rates are compared to the ones calculated by the SAILOR simulation. The results of such comparison, plotted in Figure 7, show the very good agreement between real and calculated DRI production and witness the goodness of the developed model.

Parameter	Min	Max
Shaft diameter	5m	7m
Shaft height	9m	11.6m
Gas temp. (°C)	900°C	1078°C
Inlet H_2	38%	70%
Inlet CO	15%	36%
Inlet CH_4	2%	10%

Table 2. Variability ranges for of the main parameters for the reduction tests utilized for the validation of the model

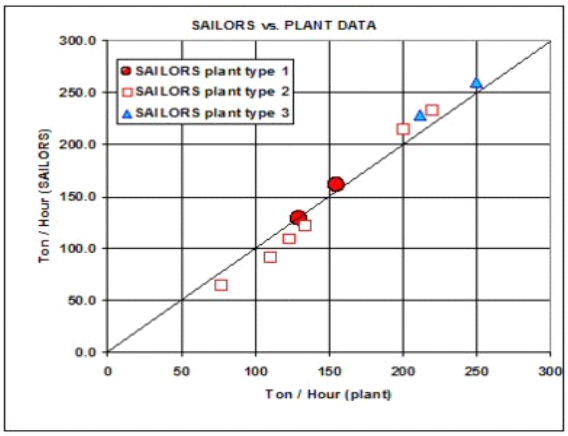

Figure 7. Comparison between calculated and actual hourly production rate of DRI for the performed tests

Conclusion and future work

SAILORS has been validated by exploiting real data coming from the most common DRI production plants which have been compared to the results of the model. The tests refer to a set of different configurations as shown in table 1. The good results obtained by the model and shown in Figure 7 encourage the use of the developed software in the designing phase of new concept DR plants.

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